Connecting via Winsock to STN

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LOGINID:ssptaeal1624

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | OCT 02 | CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt |
| NEWS 3 | OCT 19 | BEILSTEIN updated with new compounds |
| NEWS 4 | NOV 15 | Derwent Indian patent publication number format enhanced |
| NEWS 5 | NOV 19 | WPIX enhanced with XML display format |
| NEWS 6 | NOV 30 | ICSD reloaded with enhancements |
| NEWS 7 | DEC 04 | LINPADOCDB now available on STN |
| NEWS 8 | DEC 14 | BEILSTEIN pricing structure to change |
| NEWS 9 | DEC 17 | USPATOLD added to additional database clusters |
| NEWS 10 | DEC 17 | IMSDRUGCONF removed from database clusters and STN |
| NEWS 11 | DEC 17 | DGENE now includes more than 10 million sequences |
| NEWS 12 | DEC 17 | TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment |
| NEWS 13 | DEC 17 | MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary |
| NEWS 14 | DEC 17 | CA/CAplus enhanced with new custom IPC display formats |
| NEWS 15 | DEC 17 | STN Viewer enhanced with full-text patent content from USPATOLD |
| NEWS 16 | JAN 02 | STN pricing information for 2008 now available |
| NEWS 17 | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS 18 | JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS 19 | JAN 28 | MARPAT searching enhanced |
| NEWS 20 | JAN 28 | USGENE now provides USPTO sequence data within 3 days of publication |
| NEWS 21 | JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS 22 | JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements |
| NEWS 23 | FEB 08 | STN Express, Version 8.3, now available |
| NEWS 24 | FEB 20 | PCI now available as a replacement to DPCI |
| NEWS 25 | FEB 25 | IFIREF reloaded with enhancements |
| NEWS 26 | FEB 25 | IMSPRODUCT reloaded with enhancements |
| NEWS 27 | FEB 29 | WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:17:45 ON 17 MAR 2008

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 1.47 | 1.47 |

FILE 'REGISTRY' ENTERED AT 17:22:08 ON 17 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 MAR 2008 HIGHEST RN 1008362-16-0
DICTIONARY FILE UPDATES: 16 MAR 2008 HIGHEST RN 1008362-16-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

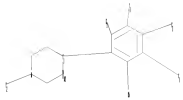
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

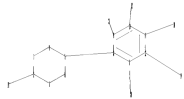
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10581591.str





chain nodes :
17 19 20 22 23 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-17 5-8 7-24 9-23 10-22 11-20 12-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-6 5-8 7-24 9-23 10-22 11-20 12-19
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

G1:C,N

G2:Cy,Ak,S

G3:X,Cy,Ak,OH,CN,NH2,NO2,H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 17:CLASS 19:CLASS 20:CLASS 22:CLASS 23:CLASS 24:Atom

L1 STRUCTURE UPLOADED

<12/04/2007> Erich Leese

```
=> d l1
L1 HAS NO ANSWERS
L1                STR
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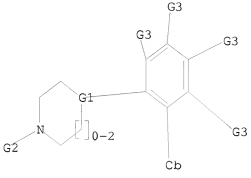


G1 C,N

G2 Cy,Ak,S

G3 X,Cy,Ak,OH,CN,NH2,NO2,H,O

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 17:23:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13611612 TO ITERATE

  1.9% PROCESSED   262703 ITERATIONS                          6 ANSWERS

  3.9% PROCESSED   525895 ITERATIONS                         11 ANSWERS

  6.4% PROCESSED   875810 ITERATIONS                         14 ANSWERS

  7.2% PROCESSED   977197 ITERATIONS                         17 ANSWERS

  7.3% PROCESSED  1000000 ITERATIONS                         17 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.01.11

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     13611612 TO 13611612
PROJECTED ANSWERS:            186 TO      276

L2           17 SEA SSS FUL L1

=>
=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             191.24     192.71

FILE 'CAPLUS' ENTERED AT 17:39:39 ON 17 MAR 2008
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FILE COVERS 1907 - 17 Mar 2008 VOL 148 ISS 12
FILE LAST UPDATED: 16 Mar 2008 (20080316/ED)

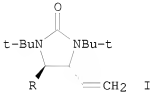
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2 full
L3 7 L2

=> d ibib abs hitstr tot

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1448274 CAPLUS
DOCUMENT NUMBER: 148:239092
TITLE: Chiral N-Heterocyclic Carbene-Pd(0)-Catalyzed Asymmetric Diamination of Conjugated Dienes and Triene
AUTHOR(S): Xu, Liang; Shi, Yian
CORPORATE SOURCE: Department of Chemistry, Colorado State University, Fort Collins, CO, 80523, USA
SOURCE: Journal of Organic Chemistry (2008), 73(2), 749-751
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

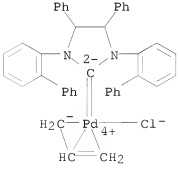



I

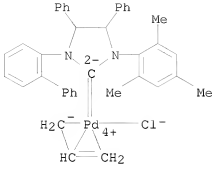
AB Studies show that a variety of conjugated dienes and triene can be enantioselectively diaminated using di-tert-butyldiaziridinone as nitrogen source and chiral N-heterocyclic carbene-Pd(0) complex as catalyst to give diamination products, e.g. I (R = Me, Et, PhCH2CH2, n-C5H11), in good enantioselectivity (62-91% ee) with high regio- and diastereoselectivity.

IT 1006064-38-5P 1006064-42-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral N-heterocyclic carbene-Pd catalysts and application to asym. diamination of conjugated dienes and triene using di-tert-butyldiaziridinone)

RN 1006064-38-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




RN 1006064-42-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1364471 CAPLUS
DOCUMENT NUMBER: 148:33768
TITLE: Preparation of bridged aryl piperazines derivatives useful for the treatment of CNS, gastrointestinal and reproductive disorders
INVENTOR(S): Creighton, Christopher John; Ross, Tina Morgan; Reitz, Allen B.; Kordik, Cheryl P.; Paget, Steven
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 122pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2007137168 | A2 | 20071129 | WO 2007-US69256 | 20070518 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| PRIORITY APPLN. INFO.: | | | US 2006-801439P | P 20060518 |
| OTHER SOURCE(S): | MARPAT 148:33768 | | | |

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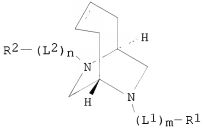


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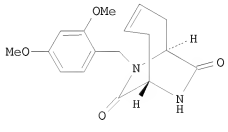



II

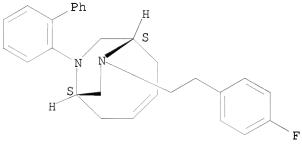
AB Title compds. represented by the formula I [wherein m = 0 or 1; L1, L2 = independently -alkyl-, -CH2-alkenyl-, -CH2-alkynyl-, etc.; R1, R2 = H, (cyclo)alkyl, aryl, etc.; n = 0 or 1; and pharmaceutically acceptable salts thereof] were prepared as serotonin transport inhibitors and/or modulators of 5HT1A. For example, II was provided in a multi-step

synthesis starting from the reaction of allylglycine Me ester with 2,4-dimethoxybenzaldehyde. I were tested for radioligand binding to the human 5-HT1A receptor and to human 5-HTT, and for [35S]GTPγS binding of 5-HT1A receptor activation and inhibition. Thus, I and their pharmaceutical compns. are useful for the treatment of depression and related disorders.

IT 959408-27-6P 959408-28-7P 959408-29-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bridged aryl piperazines derivs. useful for treatment of CNS, gastrointestinal and reproductive disorders)

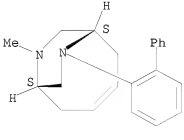
RN 959408-27-6 CAPLUS
CN 7,9-Diazabicyclo[4.2.2]dec-3-ene, 7-[1,1'-biphenyl]-2-yl-9-[2-(4-fluorophenyl)ethyl]-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.



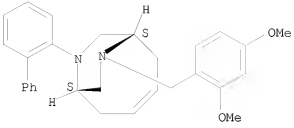

RN 959408-28-7 CAPLUS
CN 7,9-Diazabicyclo[4.2.2]dec-3-ene, 7-[1,1'-biphenyl]-2-yl-9-methyl-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.




RN 959408-29-8 CAPLUS
CN 7,9-Diazabicyclo[4.2.2]dec-3-ene, 7-[1,1'-biphenyl]-2-yl-9-[(2,4-dimethoxyphenyl)methyl]-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.


H
S
OMe
N
N
Ph
S
H
OMe

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1215849 CAPLUS
DOCUMENT NUMBER: 147:486339
TITLE: Preparation of substituted 4-piperidinylmethyl phenylmethyl ethers as NK-1 and serotonin transporter inhibitors
INVENTOR(S): Denhart, Derek J.; Degnan, Andrew P.; Tora, George O.; Han, Ying; Ramkumar, Rajamani; Ditta, Jonathan L.; Gillman, Kevin W.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 246pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2007121389 | A2 | 20071025 | WO 2007-US66682 | 20070416 |
| WO 2007121389 | A3 | 20080221 | | |
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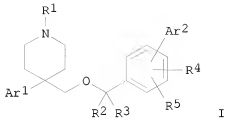
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA | | | |
| US 2007249607 | A1 | 20071025 | US 2007-734809 | 20070413 |
| PRIORITY APPLN. INFO.: | | | US 2006-792604P P | 20060417 |
| | | | US 2007-734809 A | 20070413 |

OTHER SOURCE(S): MARPAT 147:486339
GI



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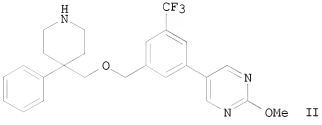


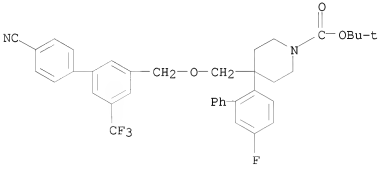
II

AB The title compds. I [R1 = H, alkyl, cycloalkyl, CH2Ph; R2, R3 = H or alkyl; R4, R5 = H, alkyl, haloalkyl, etc.; Ar1 = (un)substituted Ph or pyridinyl; Ar2 = (un)substituted Ph, naphthyl, furanyl, etc.], useful in treating disorders associated with an excess or imbalance of tachykinins or serotonin or both, were prepared E.g., a multi-step synthesis of II, starting from 4-phenyl-4-piperidinecarboxylic acid p-methylbenzenesulfonate, was given. II showed IC50 of 0.01-100 nM when tested in NK-1 binding assay and in serotonin transporter binding assay. Pharmaceutical composition comprising the compound I is disclosed.

IT 954123-38-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted 4-piperidinylmethyl phenylmethyl ethers as NK-1 and serotonin transporter inhibitors)

RN 954123-38-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[4'-cyano-5-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]methyl]-4-(5-fluoro[1,1'-biphenyl]-2-yl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1213121 CAPLUS
DOCUMENT NUMBER: 147:502389
TITLE: Preparation of diketo-piperazine and piperidine derivatives as antiviral agents
INVENTOR(S): Wang, Tao; Kadow, John F.; Zhang, Zhongxing; Yin, Zhiwei; Meanwell, Nicholas A.; Regueiro-Ren, Alicia; Swidorski, Jacob; Han, Ying; Carini, David J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S. Pat. Appl. Publ., 277pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 2007249579 | A1 | 20071025 | US 2007-733283 | 20070410 |
| WO 2007127635 | A2 | 20071108 | WO 2007-US66700 | 20070416 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |

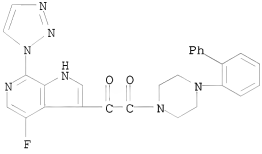
PRIORITY APPLN. INFO.: US 2006-794700P P 20060425
US 2006-794703P P 20060425
US 2007-733283 A 20070410
OTHER SOURCE(S): MARPAT 147:502389
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

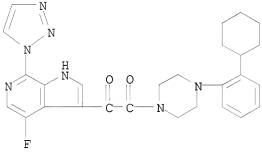
AB Title compds. I [Ring A = (un)substituted 6-membered aryl or nitrogen heteroaryl; R1 = H, alkyl or fluoroalkyl; R2 = H; R3-10 independently = H or (un)substituted alkyl; Y = (un)substituted Ph, monocyclic heteroaryl, bicyclic aryl, etc.; Z = alkyl, alkoxy, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as antiviral agents. Thus, e.g., II was prepared by Friedel-Craft acylation of 7-bromo-4-fluoro-1H-pyrrolo[2,3-c]pyridine with Me chlorooxoacetate followed by amidation with 1-(1-phenyl-1H-tetrazol-5-yl)piperazine (preparation given). In particular, the disclosure is concerned with diketo piperazine and piperidine derivs. that possess unique antiviral activity. EC50 values were determined for I with results reported in ranges with one group possessing EC50 values of ≤ 0.5 μM and the other as > 0.5 μM. More particularly, the present disclosure relates to compds. useful for the treatment of HIV and AIDS.

IT 955045-27-9P 955045-64-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diketo-piperazine and piperidine derivs. as antiviral agents)

RN 955045-27-9 CAPLUS
CN 1,2-Ethanedione, 1-(4-[1,1'-biphenyl]-2-yl-1-piperazinyl)-2-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)



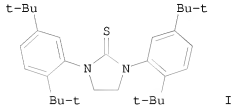
RN 955045-64-4 CAPLUS
CN 1,2-Ethanedione, 1-[4-(2-cyclohexylphenyl)-1-piperazinyl]-2-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)



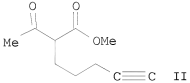
L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1026919 CAPLUS
DOCUMENT NUMBER: 147:502036
TITLE: Bulky thioureas as new ligands for gold(I)-catalyzed cyclization of acetylenic 1,3-dicarbonyl compounds
AUTHOR(S): Pan, Jie-Hui; Yang, Min; Gao, Qiang; Zhu, Nian-Yong; Yang, Dan
CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong, Hong Kong, Peop. Rep. China
SOURCE: Synthesis (2007), (16), 2539-2544
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

GI




I

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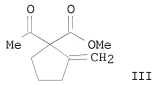


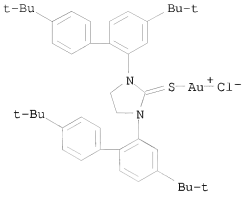

III

AB We illustrate the first use of bulky N,N'-disubstituted cyclic thioureas, e.g. I, as ligands for gold(I) catalysis. X-ray crystal structures of the thiourea-gold(I) complexes presented important information about the nature of the complexation. These complexes were found to be active catalysts for the cyclization of 1,3-dicarbonyl compds. with alkynes (Conia-ene reaction). Various acetylenic 1,3-dicarbonyl compds. underwent cycloisomerization to give mono- and bicyclic olefinic cyclopentanes in the presence of one mol% of a thiourea-gold(I) chloride complex and silver triflate. E.g., gold(I)-catalyzed cyclization of acetylenic 1,3-dicarbonyl compound II gave 96% cyclopentane derivative III.

IT 955083-84-8P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(bulky thioureas as ligands for gold(I)-catalyzed cyclization of acetylenic 1,3-dicarbonyl compds.)

RN 955083-84-8 CAPLUS

CN Gold, [1,3-bis[4,4'-bis(1,1-dimethylethyl)[1,1'-biphenyl]-2-yl]-2-imidazolidinethione-κS2]chloro- (CA INDEX NAME)



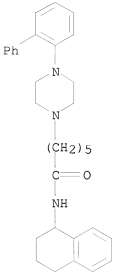

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:806254 CAPLUS
DOCUMENT NUMBER: 147:385945
TITLE: Structure-Activity Relationship Study on N-(1,2,3,4-Tetrahydronaphthalen-1-yl)-4-aryl-1-piperazinehexanamides, a Class of 5-HT7 Receptor Agents. 2
AUTHOR(S): Leopoldo, Marcello; Lacivita, Enza; Contino, Marialessandra; Colabufo, Nicola A.; Berardi, Francesco; Perrone, Roberto
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy
SOURCE: Journal of Medicinal Chemistry (2007), 50(17), 4214-4221
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:385945

AB Here the authors report the synthesis of N-(1,2,3,4-tetrahydronaphthalen-1-yl)-4-aryl-1-piperazinehexanamides 16-29 that were designed to elucidate both structure-affinity and -activity relations for the 5-HT7 receptor, by targeting the substituent in 2-position of the aryl linked to the piperazine ring. The affinities of 16-29 for 5-HT7, 5-HT1A, 5-HT2A, and D2 receptors were assessed by radioligand binding assays. The intrinsic activities at the 5-HT7 receptor of the most potent compds. were determined Substituents covering a wide range of electronic, steric, and polar properties were evaluated, revealing a key role on 5-HT7 receptor affinity and intrinsic activity. Certain lipophilic substituents (SCH3, CHMe2, NMe2, CH3, Ph) led to high-affinity agonists, whereas OH and NHCH3 substituents switched intrinsic activity toward antagonism. 4-[2-(1-Methylethyl)phenyl]-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (19), 4-(2-diphenyl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (21), and 4-(2-dimethylaminophenyl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (22) were identified as potent 5-HT7 receptor agonists (Ki = 0.13-1.1 nM, EC50 = 0.90-1.77 μM), showing selectivity over 5-HT1A, 5-HT2A, and D2 receptors.

IT 950685-64-0P, 4-(Biphenyl-2-yl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide dihydrochloride
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity relationship for N-(1,2,3,4-tetrahydronaphthalen-1-yl)-4-aryl-1-piperazinehexanamides as a class of selective 5-HT7 receptor agents)

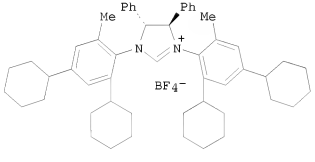
RN 950685-64-0 CAPLUS
CN 1-Piperazinehexanamide, 4-[1,1'-biphenyl]-2-yl-N-(1,2,3,4-tetrahydro-1-naphthalenyl)-, hydrochloride (1:2) (CA INDEX NAME)




●2 HCl

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:800288 CAPLUS
DOCUMENT NUMBER: 147:343686
TITLE: New N-Heterocyclic Carbene Ligand and Its Application in Asymmetric Nickel-Catalyzed Aldehyde/Alkyne Reductive Couplings
AUTHOR(S): Chaulagain, Mani Raj; Sormunen, Grant J.; Montgomery, John
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Journal of the American Chemical Society (2007), 129(31), 9568-9569
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:343686
GI




I

AB A new chiral N-heterocyclic carbene ligand (I) has been prepared and examined in nickel-catalyzed, asym. reductive couplings of aldehydes and alkynes. In comparison with related structures that have been largely examined in asym. ring-closing metathesis reactions, the new ligand provides superior yields and enantioselectivities in the nickel-catalyzed reductive couplings. The scope of asym. couplings in intermol. variants as well as a 14-membered macrocyclization is illustrated.

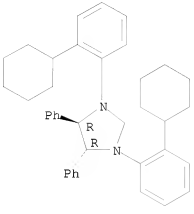
IT 948892-06-6P 948892-13-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral imidazolium ligands via coupling of chiral diamines with aryl or cyclohexyl bromide followed by cyclization for use in asym. coupling reactions)

RN 948892-06-6 CAPLUS
CN 1H-Imidazolium, 1,3-bis(2-cyclohexylphenyl)-4,5-dihydro-4,5-diphenyl-, (4R,5R)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 948892-05-5
CMF C39 H43 N2

Absolute stereochemistry.




ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

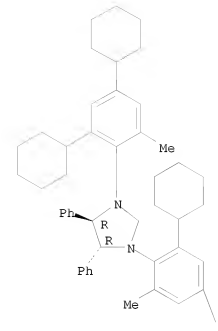

RN 948892-13-5 CAPLUS
CN 1H-Imidazolium, 1,3-bis(2,4-dicyclohexyl-6-methylphenyl)-4,5-dihydro-4,5-diphenyl-, (4R,5R)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 948892-12-4
CMF C53 H67 N2

Absolute stereochemistry.

PAGE 1-A




PAGE 2-A

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS


IT 948892-29-3
RL: CAT (Catalyst use); USES (Uses)

(stereoselective preparation of alkenyl silyl ethers via nickel catalyzed coupling of aldehydes with alkynes in the presence of triethylsilane and chiral imidazolium ligands)

RN 948892-29-3 CAPLUS

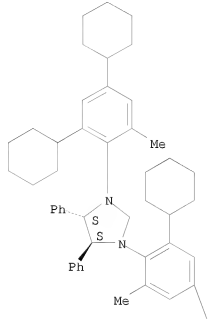
CN 1H-Imidazolium, 1,3-bis(2,4-dicyclohexyl-6-methylphenyl)-4,5-dihydro-4,5-diphenyl-, (4S,5S)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 948892-28-2
CMF C53 H67 N2

Absolute stereochemistry.

PAGE 1-A




PAGE 2-A

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14874-70-5

CMF B F4
CCI CCS

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2           17 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 17:39:39 ON 17 MAR 2008
L3            7 S L2 FULL

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    40.07     232.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -5.60      -5.60

STN INTERNATIONAL LOGOFF AT 17:41:47 ON 17 MAR 2008
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